TITLE	DESIGN OF HYBRID POWER GENERATION CYCLES EMPLOYING AMMONIA-WATER-CARBON DIOXIDE MIXTURES.
PI:	Ashish Gupta
INSTITUTION:	University at Buffalo Department of Chemical Engineering Buffalo, NY 14260 Phone: (716) 645-2911 x2221 Fax: (716) 645-3822 ashishgbuffalo.edu
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ABSTRACT

A *power cycle* generates electricity from the heat of combustion of *fossil fuels*. Its *efficiency* is governed by the cycle configuration, the operating parameters, and the working fluid. Typical designs use pure water as the fluid. In the last two decades, hybrid cycles based on *ammonia-water*, and *carbon-dioxide* mixtures as the working fluid have been proposed. These cycles may improve the power generation efficiency of Rankine cycles by 15%. Improved efficiency is important for two reasons: it lowers the cost of electricity being produced, and by reducing the consumption of fossil fuels per unit power, it reduces the generation of environmental pollutants.

The goal of this project is to develop a computational optimization-based method for the design and analysis of hybrid bottoming power cycles to minimize the usage of fossil fuels. The development of this methodology has been achieved by formulating this task as that of selecting the least cost power cycle design from all possible configurations. We employ a detailed thermodynamic property prediction package we have developed under a DOE-FETC grant to model working fluid mixtures. Preliminary results from this work suggest that a pure NH_3 cycle outperforms steam or the expensive Kalina cycle.

The lack of a unified framework to systematically develop cycle design alternatives results in missed opportunities. Hence, for process representation, we propose *a new graph theoretic approach to power cycle design.* The **key feature** of this representation is that it reformulates the nonconvex problems (with multiple minima) that result from an *optimization based formulation of the power cycle synthesis task* as a linear program which can be solved globally. We have applied this method to save energy costs in other chemical process design problems, such as in liquid-liquid extraction, and in air separation.

This work in progress provides the basis for a general method to evaluate and design *Vision 21 plant configurations*. Though bottoming cycles are only a component of the energy-plex, our design methodology can be modified to design the entire complex with water-gas shift reactions, fuel cells, and gas turbine cycles. The proposed innovative concept work will develop this capability for this component of the Vision 21 plant: the bottoming cycle to recover heat from the stack gases. a 10% improvement in fossil fuel power plant efficiency may lead to a 5% increase in U.S. power generation capacity, without any increase in fuel consumption.

Presentations and Student Support

Journal Articles (Peer Reviewed)

1. Patra, A. and Gupta, A. "A Systematic Strategy For Simultaneous Adaptive *hp* Finite Element Mesh Modification Using Nonlinear Programming," *J. Applied Comp. Mech.*, 190 (2001), 3797-3818.

2. Sourlas, D.D. and A. Gupta *A Pollution Prevention Course for the Chemical Engineering Curriculum.* Chemical Engineering Education in the New Millenium, Topical Conference Proceedings, AIChE Annual Meeting, Editors: R.P. Hesketh, C.S. Howat and D.S. Dixon, pp. 662-675, November 12-17, 2000, Los Angeles, CA.

Conference Presentations

1. Gupta, A. (Invited) *A Graph Theoretic Approach to Process Synthesis.* Praxair Seminar Series, Industrial Engineering Department, University at Buffalo, NY, December 2000.

2. Gupta, A., *A Graph Theoretic Approach to Process Synthesis.* FMC Technical Center, Tonawanda, NY, November 2000.

3. Gupta, A. and Sourlas, D.D., *Minimum Utility Bounds For Liquid-Liquid Extraction Systems.* Paper #49g. AIChE Annual Meeting, Los Angeles, CA, November 2000.

4. Gupta, A. and D.D. Sourlas (Speaker), *A Pollution Prevention Course for the Chemical Engineering Curriculum.* Paper #67f. AIChE Annual Meeting, Los Angeles, CA, November 2000.

5. Gupta, A., *A Graph Theoretic Approach to Mixed Fluid Power Cycle Synthesis.* Paper #242i. AIChE Annual Meeting, Los Angeles, CA, November 2000.

6. Gupta, A. (Speaker) and A. Patra, *Solution of Reaction Diffusion Equations Through Systematically Modified Adaptive hp Meshes.* Paper #272j. AIChE Annual Meeting, Los Angeles, CA, November 2000.

7. Gupta, A. (Speaker) and A. Patra, *Solution of Reaction-Diffusion Equations With A Systematic Adaptive hp Finite Element Mesh Modification Strategy.* First SIAM Computational Science and Engineering Meeting, September 2000. Two presentations.

8. Gupta, A., *A Graph Theoretic Approach to Synthesis of Reactive Distillation Systems.* Gordon Research Conference on Separations & Purifications, August 2000.

Students Supported Under This Grant

- Ananda Viraha Venkata, graduate student, 1/2001-3/2001, in Chemical Engineering, University at Buffalo